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Reactive Transport Modelling By Using Eulerian-Lagrangian Methods Based on Mixing

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Abstract:

Reactive transport use to be a complicated problem by the difficulty of finding a universal numerical method, which reproduces the natural behaviour. Eulerian methods provide accurate results, since they give second order convergence, but they require meeting stability conditions that restrict their actual applicability. Eulerian - Lagrangian methods overcome these limitations, but often cause additional mixing by numerical dispersion. This is a particularly serious problem when transport is coupled to fast chemical reactions, whose rate is controlled by mixing.

This work proposes an Eulerian-Lagrangian method without numerical dispersion for solving reactive transport based on mixing. The method consists on the construction of a streamline oriented grid such that the transit time between sequential cells remains constant (isochronal mesh). We have tested the method performances in two different cases: 1) Instantaneous point injection with analytical solution and 2) considering an isolated fracture. In both we have compared the proposed method against existing Eulerian and Eulerian-Lagrangian methods. The results confirm that the proposed method is superior to the two existing cases where dispersivities are medium and low, although the method needs additional refinements in mediums with great heterogeneous. In addition, a new reactive transport method has been obtained.